Plasma Phase Transition in Dense Hydrogen and Electron-Hole Plasmas

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Plasma phase transitions (PPT) in dense hydrogen and electron-hole plasmas are investigated by direct path integral Monte Carlo methods (DPIMC). The phase boundary of the electron-hole liquid in Germanium is calculated and is found to agree reasonably well with the known experimental results. Analogous results are found for high-density hydrogen. For a temperature of $T = 10,000K$ it is shown that the internal energy is lowered due to droplet formation for densities between $10^{23} cm^{-3}$ and $10^{24} cm^{-3}$.

1. Path integral Monte Carlo simulations

All thermodynamic properties of a two-component plasma are defined by the partition function Z which, for the case of N_e electrons and N_p protons, is given by $Z(N_e, N_p, V, \beta) = \frac{Q(N_e,N_p,\beta)}{N_e! N_p!}$, with $Q(N_e, N_p, \beta) = \sum_\sigma \int_V dq\, dr\, \rho(q, r, \sigma; \beta)$, where $\beta = 1/k_B T$. The exact density matrix is, for a quantum system, in general, not known but can be constructed using a path integral representation [1, 2] $\int_V dR^{(0)} \sum_\sigma \rho(R^{(0)}, \sigma; \beta) = \int_V dR^{(0)} \dots dR^{(n)}\, \rho^{(1)} \cdot \rho^{(2)} \dots \rho^{(n)} \times \sum_\sigma \sum_P (\pm 1)^{\kappa_P} \mathcal{S}(\sigma, \hat{P}\sigma')\, \hat{P} \rho^{(n+1)}$, where $\rho^{(i)} \equiv \rho\left(R^{(i-1)}, R^{(i)}; \Delta\beta\right) \equiv \langle R^{(i-1)} | e^{-\Delta\beta \hat{H}} | R^{(i)} \rangle$, whereas $\Delta\beta \equiv \beta/(n+1)$ and $\Delta\lambda_a^2 = 2\pi\hbar^2 \Delta\beta / m_a$, $a = p, e$. $\hat{H}$ is the Hamilton operator, $\hat{H} = \hat{K} + \hat{U}_c$, containing kinetic and potential energy contributions, $\hat{K}$ and $\hat{U}_c$, respectively, with $\hat{U}_c = \hat{U}_c^p + \hat{U}_c^e + \hat{U}_c^{ep}$ being the sum of the Coulomb potentials between protons (p), electrons (e) and electrons and protons (ep). Further, σ comprises all particle spins, and the particle coordinates are denoted by $R^{(i)} = (q^{(i)}, r^{(i)}) \equiv (R_p^{(i)}, R_e^{(i)})$, for $i = 1, \dots n+1$, $R^{(0)} \equiv (q, r) \equiv (R_p^{(0)}, R_e^{(0)})$, and $R^{(n+1)} \equiv R^{(0)}$ and $\sigma' = \sigma$. This means, the particles are represented by fermionic loops with the coordinates (beads) $[R] \equiv [R^{(0)}; R^{(1)}; \dots; R^{(n)}; R^{(n+1)}]$, where q and r denote the electron and proton coordinates, respectively. The spin gives rise to the spin part of the density matrix $\mathcal{S}$, whereas exchange effects are accounted for by the permutation operator $\hat{P}$, which acts on the electron coordinates and spin projections, and the sum over the permutations with parity κ_P. To compute thermodynamic functions, the logarithm of the partition function has to be differentiated with respect to thermodynamic variables, so for internal energy E we have $\beta E = -\beta \partial \ln Q / \partial \beta$

2. Numerical Results

Since the PPT in dense hydrogen is still hypothetical and has not been observed experimentally, it is reasonable to look for other systems where similar conditions exist. A suitable example is electron-hole plasma in low-temperature semiconductors, for which droplet formation is well established and observed ex-

perimentally three decades ago [3]. We, therefore, performed DPIMC simulations for electron hole plasmas. Below the critical temperature the simulations exhibit anomalously large fluctuations and an unstable behavior of the pressure. The e-h-plasma is found to phase separate and form large droplets. The phase boundary of the electron-hole liquid (e-h-droplets) in Germanium obtained by our DPIMC method is presented in Fig. 1 together with the experimental data. We observe good agreement. Deviations may be connected with complex band structure of Germanium approximated in our simulations by a two-band parabolic mass model.

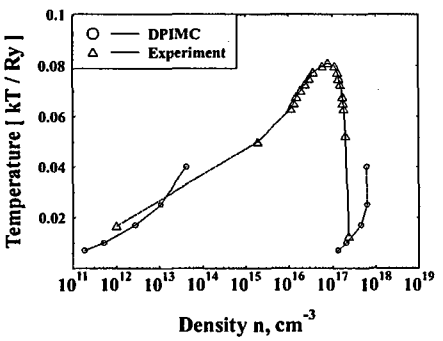

Figure 1: Phase boundary of the electron-hole liquid in bulk Germanium. Experiment - [3]. Temperature is presented in units of the exciton binding energy.

Fig.2 presents results of our calculations for pressure and energy of hydrogen at $T = 10,000K$, which is well below the critical point of the PPT predicted by chemical models (around $T = 15,000$K). In our calculations between 10^{22}cm^{-3} and 10^{24}cm^{-3} calculated pressure becomes negative. We find also that in this region plasma energy is systematically lower than the RPIMC results [4]. If average distance between plasma particles is of the order of the size of a hydrogen molecule the homogeneous plasma state becomes unstable, and many-particle clusters appear. Results of one independent well tested method based on density functional theory (DFT) are presented on Fig. 2, where PPT was obtained at smaller density [5].

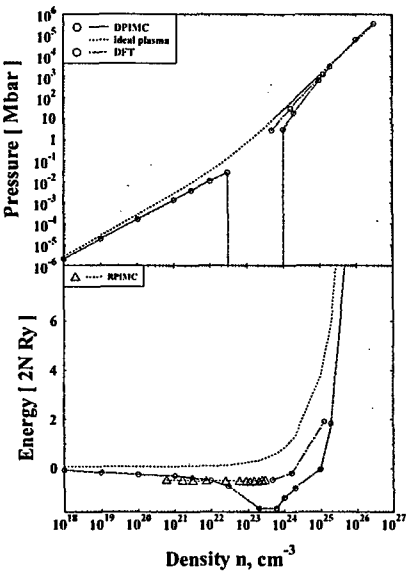

Figure 2: Pressure and energy of hydrogen for $T = 10,000K$, DFT - [5], RPIMC - [4].

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